The "topological" charge for the finite XX quantum chain

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Abstract. It is shown that an operator (in general non-local) commutes with the Hamiltonian describing the finite XX quantum chain with certain non-diagonal boundary terms. In the infinite volume limit this operator gives the "topological" charge.

We consider the L sites XX quantum chain with non-diagonal boundary terms given by the Hamiltonian:

$$H = \frac{1}{4}\sum_{j=1}^{L-1}\left(\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y\right) + \lambda\sigma_1^x + \mu\left[\cos(\chi)\sigma_L^x - \sin(\chi)\sigma_L^y\right] \tag{1}$$

here λ, μ and χ are parameters. Obviously the $O(2)$ symmetry on the bulk terms is broken by the boundary terms. The question is if this finite quantum chain has no "hidden" symmetries (hidden symmetries occur normally in the thermodynamic limit only). We will show that it does. In order to understand the problem and find the "hidden" symmetries, it is convenient [1] to add two more sites denoted with 0 and $L+1$ and consider another Hamiltonian that we denote by

$$H_{\rm f} = \frac{1}{4}\sum_{j=1}^{L-1}\left(\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y\right) + \lambda\sigma_0^x\sigma_1^x + \mu\left[\cos(\chi)\sigma_L^x\sigma_{L+1}^x - \sin(\chi)\sigma_L^y\sigma_{L+1}^x\right]. \tag{2}$$

(in Refs. [2, 3] $H_{\rm f}$ was denoted by $H_{\rm long}$). Notice that $H_{\rm f}$ is $Z(2)\times Z(2)$ symmetric since the matrices σ_0^x and σ_{L+1}^x commute with $H_{\rm f}$. Therefore the spectrum of $H_{\rm f}$ decomposes into four blocks $(\pm,\pm),(\pm,\mp)$ corresponding to the eigenvalues ±1 of the σ^x matrices. The Hamiltonian H given by eq.(1) corresponds to the $(+,+)$ block. Actually the symmetry of $H_{\rm f}$ is larger than $Z(2)\times Z(2)$, it is the finite non-abelian group with the three generators $\sigma_0^x, \sigma_{L+1}^x$ and $U = \sigma_0^z\sigma_1^z\cdots\sigma_{L+1}^z$ (which also commutes with $H_{\rm f}$). Moreover using the obvious relations:

$$\{\sigma_0^x, U\} = \{\sigma_{L+1}^x, U\} = 0; \qquad U^2 = 1 \tag{3}$$

one can show that if $|\mu,\nu,E\rangle$ is an eigenvector of $H_{\rm f}$ in the (μ,ν) sector, corresponding to the eigenvalue E, then

$$U \mid \mu,\nu,E\rangle = \mid -\mu,-\nu,E\rangle \tag{4}$$

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is also an eigenvector of $H_{\rm f}$, in the $(-\mu,-\nu)$ sector corresponding to the same eigenvalue E. As a result, the whole spectrum of $H_{\rm f}$ is doubly degenerate: the spectra in the sectors $(+,+)$ and $(-,-)$ (respectively $(+,-)$ and $(-,+)$) are identical. Since the degeneracy includes the ground-state, the symmetry is spontaneously broken. The Hamiltonian $H_{\rm f}$ can be diagonalized in terms of free fermions which does not mean that the fermionic energies or the wave functions are simple to derive since the secular equation is hard to solve. This problem is discussed in detail in Ref.[2]. Moreover, for our purpose one needs to find boundary terms which lead to fermionic energies of a special form (the reason is going to be explained shortly), therefore from our collection of boundary terms where we could find solutions of the secular equation, we will consider only two kinds of boundary conditions:

- $\lambda = \mu = \dfrac{1}{\sqrt{8}}$ (5)
- $\lambda = \mu = \dfrac{1}{4}; \qquad \chi = 0$ (6)

We have to consider the cases L odd and even separately. The reason is the following one: for L odd the ground-state of $H_{\rm f}$ is in the $(+,+)$ sector in which we are interested. For L even the ground-state is in the $(+,-)$ sector. Since we are more interested in the spectra where the ground-state is, we will confine ourselves to the case L odd (as opposed to the case of diagonal boundary terms where the ground-state appears in chains with an even number of sites [4]). One can repeat the whole procedure described below for L even. For both cases (5) and (6) one finds a zero fermionic mode which explains in a different way why each level of $H_{\rm f}$ is doubly degenerate. We now specialize to the boundary condition (5). The energy gaps are given [2] by the fermionic energies (the zero mode not included)

$$\Lambda_n^{\pm} = \sin\left(\frac{2n+1}{L+1}\frac{\pi}{2} \pm \frac{\chi}{L+1}\right) \qquad 0 \leq n \leq (L-1)/2 \tag{7}$$

It is convenient to consider the operator

$$T_{\rm f} = \frac{1}{2}\sum_{n=0}^{(L-1)/2}(N_n^+ - N_n^-). \tag{8}$$

where $N_n^{\pm}$ are fermionic number operators ($N_n^{\pm} = 0, 1$) corresponding to the energies given by eq.(7). The eigenvalues of $T_{\rm f}$ denoted by m are obviously given by integer or half-integer numbers. Obviously this allows a $Z(2)$ grading. It turns out [2] that in the $(+,+)$ sector m takes integer values (even number of fermions) whereas in the $(+,-)$ sector it takes half-integer values (odd number of fermions). We define the partition function corresponding to the eigenvalue m of $T_{\rm f}$, for a chain with L sites

$$Z_m(L) = {\rm tr}\, z^{\frac{L}{\pi}\left[\sum_{n=0}^{(L-1)/2}\left(\Lambda_n^+ N_n^+ + \Lambda_n^- N_n^-\right)\right]} \tag{9}$$

with the constraint

$$\frac{1}{2}\sum_{n=0}^{(L-1)/2}(N_n^+ - N_n^-) = m \tag{10}$$

and consider the sectors $(+,+)$ and $(+,-)$ only. In the thermodynamic limit one obtains:

$$Z_m = \lim_{L\to\infty} Z_m(L) = z^{2(m+\chi/(2\pi))^2 - \chi^2/(2\pi^2)} \prod_{n=1}^{\infty} (1-z^n)^{-1} \tag{11}$$

which is what one would expect if T_{f} corresponds to the "topological" charge. If we consider the $(+,+)$ sector (which as mentioned corresponds to the original Hamiltonian given by eq.(1)) and sum over m integer the partition functions given by eq.(11), one gets the known partition function for a compactified bosonic field (with the correct radius) and von Neumann boundary conditions at both ends [3, 5, 6]. Actually the whole algebraic structure of the problem, in the thermodynamic limit, can be read-off from the expressions (7):

$$\lim_{L\to\infty} \left(\frac{L}{\pi} \Lambda_n^{\pm} \right) = n + 1/2 \pm \chi/\pi \tag{12}$$

if we keep in mind that the sum of two integer numbers is an integer number. One could pursue this issue further and make contact with the sine-Gordon model with a boundary at the free fermion point where much work was done [7, 8, 9]. In this paper we are however interested in the properties of the finite chain given by eq.(1) and want therefore to get the "topological" charge T for this chain. In order to do so, we have to write T_{f} given by eq.(8) in the basis where H_{f} is written (see eq.(2)) and project on the $(+,+)$ sector. This is a lengthy calculation where we have used the results of Ref.[2]. One obtains

$$\begin{aligned}
T = \frac{-1}{4L+4} \sum_{\substack{k,j=1\\ k+j\ \mathrm{odd}\\ k<j}}^{L} \Bigg\{ & \\
& \left[f(j-k)\cos(\chi\frac{k-j}{L+1}) - (-1)^k f(k+j)\cos(\chi\frac{k+j}{L+1}) \right] \sigma_k^y \sigma_{k+1}^z \cdots \sigma_{j-1}^z \sigma_j^x \\
& - \left[f(j-k)\cos(\chi\frac{k-j}{L+1}) + (-1)^k f(k+j)\cos(\chi\frac{k+j}{L+1}) \right] \sigma_k^x \sigma_{k+1}^z \cdots \sigma_{j-1}^z \sigma_j^y \\
& + \left[f(j-k)\sin(\chi\frac{k-j}{L+1}) + (-1)^k f(k+j)\sin(\chi\frac{k+j}{L+1}) \right] \sigma_k^y \sigma_{k+1}^z \cdots \sigma_{j-1}^z \sigma_j^y \\
& + \left[f(j-k)\sin(\chi\frac{k-j}{L+1}) - (-1)^k f(k+j)\sin(\chi\frac{k+j}{L+1}) \right] \sigma_k^x \sigma_{k+1}^z \cdots \sigma_{j-1}^z \sigma_j^x \Bigg\} \\
& + \frac{1}{\sqrt{8}(L+1)} \sum_{\substack{j=1\\ j\ \mathrm{odd}}}^{L} \Bigg\{ f(j)\cos(\chi\frac{j}{L+1}) \sigma_1^z \cdots \sigma_{j-1}^z \sigma_j^y \\
& f(j)\sin(\chi\frac{j}{L+1}) \sigma_1^z \cdots \sigma_{j-1}^z \sigma_j^x - f(j+L+1)\cos(\chi\frac{j}{L+1}) \sigma_j^y \sigma_{j+1}^z \cdots \sigma_L^z \\
& - f(j+L+1)\sin(\chi\frac{j}{L+1}) \sigma_j^x \sigma_{j+1}^z \cdots \sigma_L^z \Bigg\}
\end{aligned} \tag{13}$$

where

$$f(x) = 1/\sin\left(\frac{x\pi}{2L+2}\right). \tag{14}$$

T is a pseudoscalar for $\chi = 0$ when H is parity invariant. One can also check that

$$[T, H] = 0 \tag{15}$$

only for L odd and not for L even. The expression (13) is horrible, what is important is that it exists. Let us stress that we were able to identify T_{f} and therefore T only because the fermionic energies had the form (7). We have not found [2] any other boundary conditions where we know the spectrum of the finite chain and where the partition functions have the form given by eq.(11) with χ different of zero (only in this case we can write T_{f} like in eq.(8)). We would have liked to have more examples in order to make sure that the boundary condition (5) is not a special case and that only for this case one can find the "topological" charge. There is however one case (given by the boundary condition (6)) where although the spectrum of the finite quantum chain H is twice degenerate (nothing to do with a zero mode but with the fact that in the continuum it gives the partition function (11) with $\chi = 0$):

$$\Lambda_n^+ = \Lambda_n^- = \sin\left(\frac{2n+1}{L+2}\frac{\pi}{2}\right) \qquad 0 \leq n \leq (L-1)/2 \tag{16}$$

we were able to identify the "topological" charge. We did it using a trick. We took $\lambda = \mu = 1/4$ and a small value for χ in eq.(2), diagonalized H_{f} numerically and identified $\Lambda_n^{\pm}$ and the creation and annihilation operators corresponding to these energy levels. This has allowed us to guess T_{f} for $\chi = 0$ where the spectrum of H_{f} is known. We found:

$$T_{\mathrm{f}} = \frac{1}{8}\sum_{j=1}^{L-1}\left[\left(1+(-1)^j\right)\sigma_j^x\sigma_{j+1}^y - \left(1-(-1)^j\right)\sigma_j^y\sigma_{j+1}^x\right] + \frac{1}{4}\left(\sigma_0^x\sigma_1^y - \sigma_L^y\sigma_{L+1}^x\right) \tag{17}$$

and

$$T = \frac{1}{8}\sum_{j=1}^{L-1}\left[\left(1+(-1)^j\right)\sigma_j^x\sigma_{j+1}^y - \left(1-(-1)^j\right)\sigma_j^y\sigma_{j+1}^x\right] + \frac{1}{4}\left(\sigma_1^y - \sigma_L^y\right). \tag{18}$$

Notice that the expressions (17) and (18) are local ones. One can look at T and consider it as a quantum chain (keep in mind that it commutes with H only for L odd). This quantum chain has amusing properties. If we disregard the boundary terms, it is trivial to diagonalize it and one obtains

$$\frac{1}{2}\left(\sum_{k=1}^{L-1} N_k\right) - \frac{L-1}{4} \tag{19}$$

here N_k are fermionic operators. If one takes into account the boundary terms, in order to diagonalize it, one has to use T_{f} given by eq.(17) and project in order to find the spectrum of T (the way we did in order to find the spectrum of H out of the spectrum of H_{f}). For L odd the spectrum is the known one (integer values) since T is the "topological" charge. For L even, the spectrum is complicated.

One can ask what we have learned from our exercise. The fact that the quantum chain (1) has many conservation laws (the total number of fermions is just one example) should not be a surprise since its spectrum is related to the one of H_{f} which is a free

system. We think that the fact that we have been able to identify the "topological" charge which is related to the magnetic charge in the Coulomb gas description or to vortices (see [10] for a review on the subject) on a finite lattice is interesting and that this identification can probably be done not only for the XX chain, but for the XXZ chain too. How to do this generalization is by no means clear to us.

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